

Methyl hexanedioate  
627-91-8 | DTXSID9044451

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.09e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.49e-01

Confidence level: 3.27e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Naphthylamine</div> <div>Measured: 4.00e-01</div> <div>Predicted: 9.37e-04</div>	<div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 3.47e-05</div> <div>Predicted: 2.39e-02</div>	<div>Image not found</div> <div>Piperophos</div> <div>Measured: 5.48e-02</div> <div>Predicted: 3.95e-07</div>
<div>Image not found</div> <div>Benazolin-ethyl</div> <div>Measured: 2.89e-07</div> <div>Predicted: 9.58e-07</div>	<div>Image not found</div> <div>Isoproturon</div> <div>Measured: 7.95e-05</div> <div>Predicted: 6.19e-08</div>	